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                 ENCOMPLIT/ENCOMPLIT2 search fields enhanced
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                 REGISTRY
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                 BEILSTEIN substance information now available on
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                 DGENE, PCTGEN and USGENE enhanced with increased
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                 limits for exact sequence match searches and
                 introduction of free HIT display format
NEWS 14
         MAY 15
                 INPADOCDB and INPAFAMDB enhanced with Chinese legal
                 status data
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         MAY 28 CAS databases on STN enhanced with NANO super role in
                 records back to 1992
NEWS 16
         JUN 01 CAS REGISTRY Source of Registration (SR) searching
                 enhanced on STN
NEWS 17
         JUN 26 NUTRACEUT and PHARMAML no longer updated
NEWS 18
         JUN 29
                 IMSCOPROFILE now reloaded monthly
NEWS 19 JUN 29 EPFULL adds SLART to AB, MCLM, and TI fields
NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
             AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.
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Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 13:48:12 ON 06 JUL 2009

=> file registry
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 2.64 2.64

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 13:55:15 ON 06 JUL 2009 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the  ${\tt ZIC/VINITI}$  data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 JUL 2009 HIGHEST RN 1160786-08-2 DICTIONARY FILE UPDATES: 3 JUL 2009 HIGHEST RN 1160786-08-2

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

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```
chain nodes :
10 11 12 13 14 15 16 37 38
ring nodes :
1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 9 \quad 17 \quad 18 \quad 19 \quad 20 \quad 21 \quad 22 \quad 23 \quad 24 \quad 25 \quad 26 \quad 27 \quad 30 \quad 31 \quad 32
33 34 39 40 41 42 43 44 46 47 48 49 50 51 52 53 54 55 56 57
chain bonds :
8-10 \quad 10-11 \quad 10-13 \quad 11-12 \quad 11-15 \quad 13-14 \quad 13-16 \quad 14-37 \quad 37-38
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 17-18 17-22 18-19 19-20 20-21
 21-22 23-24 23-27 24-25 25-26 26-27 30-31 30-34 31-32
                                                                       32-33 33-34 39-40
 39-44 40-41 41-42 42-43 43-44 46-47 46-51 47-48 48-49
                                                                       49-50 50-51
 52-57 53-54 54-55 55-56 56-57
exact/norm bonds :
5-7 6-9 7-8 8-9 8-10 11-12 11-15 13-14 13-16 14-37 23-24 23-27 24-25
25-26 26-27 30-31 30-34 31-32 32-33 33-34 37-38
exact bonds :
10-11 10-13
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 17-18 \quad 17-22 \quad 18-19 \quad 19-20 \quad 20-21 \quad 21-22 \quad 39-40
39-44 40-41 41-42 42-43 43-44 46-47 46-51 47-48 48-49 49-50 50-51 52-53
52-57 53-54 54-55 55-56 56-57
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom

19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 37:CLASS 38:CLASS 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom

51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 57:Atom

G1:[\*1],[\*2],[\*3]

Match level:

G2:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6]

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STF

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s sam 11

SAMPLE SEARCH INITIATED 13:57:48 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

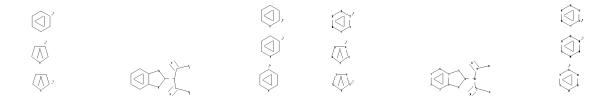
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 0 TO 0 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=>

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chain nodes :

10 11 12 13 14 15 16

ring nodes :

chain bonds : 8-10 10-11 10-13 11-12 11-15 13-14 13-16 ring bonds :  $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-9 \quad 7-8 \quad 8-9 \quad 17-18 \quad 17-22 \quad 18-19 \quad 19-20 \quad 20-21$  $21 - 22 \quad 23 - 24 \quad 23 - 27 \quad 24 - 25 \quad 25 - 26 \quad 26 - 27 \quad 30 - 31 \quad 30 - 34 \quad 31 - 32 \quad 32 - 33 \quad 33 - 34 \quad 37 - 38 \quad 33 - 34 \quad 37 - 38 \quad 33 - 34 \quad 37 - 38 \quad 37 -$ 37-42 38-39 39-40 40-41 41-42 44-45 44-49 45-46 46-47 47-48 48-49 50-5150-55 51-52 52-53 53-54 54-55 exact/norm bonds : 5-7 6-9 7-8 8-9 8-10 11-12 11-15 13-14 13-16 23-24 23-27 24-25 25-26 26-27 30-31 30-34 31-32 32-33 33-34 exact bonds : 10-11 10-13 normalized bonds :  $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 17-18 \quad 17-22 \quad 18-19 \quad 19-20 \quad 20-21 \quad 21-22 \quad 37-38$ 37-42 38-39 39-40 40-41 41-42 44-45 44-49 45-46 46-47 47-48 48-49 50-5150-55 51-52 52-53 53-54 54-55

G1:[\*1],[\*2],[\*3]

G2:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6]

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom

50 ANSWERS

L3 STRUCTURE UPLOADED

=> s 13

SAMPLE SEARCH INITIATED 14:03:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 78 TO ITERATE

100.0% PROCESSED 78 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 1031 TO 2089
PROJECTED ANSWERS: 964 TO 1996

L4 50 SEA SSS SAM L3

=> d sca

L4 50 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Propanimidamide, N-[[3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(2-dihydro-2H-benzimidazol-2-ylidene)]

methylphenyl)-1,3-dioxopropyl]phenyl]sulfonyl]-2-hydroxy-, (2R)-

MF C26 H24 N4 O5 S

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L4 50 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Butanimidamide, N-[[3-[3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxopropyl]phenyl]sulfonyl]-4,4,4-trifluoro-2-oxo-
- MF C26 H17 F5 N4 O5 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

MF C26 H22 F2 N4 O4 S

Double bond geometry as shown.

PAGE 1-A

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Propanimidamide, N-[[5-[3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxopropyl]-2-fluorophenyl]sulfonyl]-2-hydroxy-, (2R)-

MF C25 H19 F3 N4 O5 S

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Propanimidamide, N-[[3-[3-(6-chloro-3-pyridiny1)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxopropy1]-2-methylpheny1]sulfony1]-2-hydroxy-2-methyl-

MF C26 H24 C1 N5 O5 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

 ${\tt L4}$  50 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Propanimidamide, N-[[3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3fluoro-2-methylphenyl)-1,3-dioxopropyl]phenyl]sulfonyl]-2-hydroxy-2-methylMF C27 H25 F N4 O5 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenesulfonyl chloride, 5-[3-(2-chloro-5-fluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxopropyl]-2-fluoro-

MF C22 H12 C12 F2 N2 O4 S

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-(3-chloro-5-fluoropheny1)-3-(3-ethenylpheny1)-2-(5-fluoro-1,3-dihydro-2H-benzimidazol-2-ylidene)-

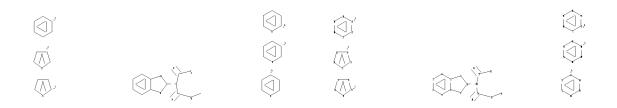
MF C24 H15 C1 F2 N2 O2

$$H_2C = CH$$
 $C = O$ 
 $C1$ 
 $C = CH$ 
 $C = O$ 
 $C1$ 
 $C = O$ 
 $C$ 

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

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10 11 12 13 14 15 16 59 ring nodes :  $1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 9 \quad 17 \quad 18 \quad 19 \quad 20 \quad 21 \quad 22 \quad 23 \quad 24 \quad 25 \quad 26 \quad 27 \quad 30 \quad 31 \quad 32$ 33 34 37 38 39 40 41 42 44 45 46 47 48 49 50 51 52 53 54 55 chain bonds :  $8-10 \quad 10-11 \quad 10-13 \quad 11-12 \quad 11-15 \quad 13-14 \quad 13-16 \quad 14-59$ ring bonds : 3-4 4-5 5-6 5-7 6-9 7-8 8-9 17-18 17-22 1-2 1-6 2-3 18-19 19-20 20-21 21-22 23-24 23-27 24-25 25-26 26-27 30-31 30-34 31-32 32-33 33-34

37-38 37-42 38-39 39-40 40-41 41-42 44-45 44-49 45-46 46-47 47-48 48-49 50-51 50-55 51-52 52-53 53-54 54-55

exact/norm bonds :

chain nodes :

10-11 10-13

normalized bonds :

G1:[\*1],[\*2],[\*3]

G2:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6]

### Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 59:CLASS

#### L5 STRUCTURE UPLOADED

=> s 15

SAMPLE SEARCH INITIATED 14:08:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 0 TO 0

PROJECTED ITERATIONS: 0 TO 0 PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=>

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```
chain nodes :
10 11 12 13 14 15 16 59
ring nodes :
1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 9 \quad 17 \quad 18 \quad 19 \quad 20 \quad 21 \quad 22 \quad 23 \quad 24 \quad 25 \quad 26 \quad 27 \quad 30 \quad 31 \quad 32
33 34 37 38 39 40 41 42 44 45 46 47 48 49 50 51 52 53 54 55
chain bonds :
8-10 10-11 10-13 11-12 11-15 13-14 13-16 14-59
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 17-18 17-22 18-19 19-20 20-21
 21-22 23-24 23-27 24-25 25-26 26-27 30-31 30-34 31-32
                                                                    32-33 33-34 37-38
 37-42 38-39 39-40 40-41 41-42 44-45 44-49 45-46 46-47
                                                                    47-48 48-49
 50-55 51-52 52-53 53-54 54-55
exact/norm bonds :
5-7 6-9 7-8 8-9 8-10 11-12 11-15 13-14 13-16 14-59 23-24 23-27 24-25
25-26 26-27 30-31 30-34 31-32 32-33 33-34
exact bonds :
10-11 10-13
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 17-18 \quad 17-22 \quad 18-19 \quad 19-20 \quad 20-21 \quad 21-22 \quad 37-38
37-42 38-39 39-40 40-41 41-42 44-45 44-49 45-46 46-47 47-48 48-49 50-51
50-55 51-52 52-53 53-54 54-55
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom

19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom

G1:[\*1],[\*2],[\*3]

Match level:

G2:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6]

51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 59:CLASS

## L7 STRUCTURE UPLOADED

=> s 17

SAMPLE SEARCH INITIATED 14:09:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 31 TO ITERATE

100.0% PROCESSED 31 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 286 TO 95

PROJECTED ITERATIONS: 286 TO 954 PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> =>

 $\label{localing c:locuments} \begin{tabular}{ll} Uploading C:\Documents and Settings\vrodriguezgarcia\My Documents\e-Red Folder\10588485\L9.str \end{tabular}$ 

chain nodes :
10 11 12 13 14 15 16 57 58 59 60 61 62 69 70 77 78 85 86 93 94
109 110 111 112
ring nodes :
1 2 3 4 5 6 7 8 9 17 18 19 20 21 22 23 24 25 26 27 30 31 32
33 34 36 37 38 39 40 41 43 44 45 46 47 48 49 50 51 52 53 54 63
64 65 66 67 71 72 73 74 75 79 80 81 82 83 87 88 89 90 91 95 96
97 98 99 100 102 103 104 105 106 107 113 114 115 116 117 118 119
120 121 122 123 124 125 126 127 128

```
chain bonds :
8-10 \quad 10-11 \quad 10-13 \quad 11-12 \quad 11-15 \quad 13-14 \quad 13-16 \quad 20-57 \quad 24-61 \quad 31-59 \quad 57-58 \quad 59-60
61-62 65-69 69-70 74-77 77-78 81-85 85-86 91-93 93-94 96-111 104-109
109-110 111-112
ring bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-9 \quad 7-8 \quad 8-9 \quad 17-18 \quad 17-22 \quad 18-19 \quad 19-20 \quad 20-21
  36-41 37-38 38-39 39-40 40-41 43-44 43-48 44-45 45-46 46-47 47-48 49-50
  49-54 50-51 51-52 52-53 53-54 63-64 63-67 64-65 65-66 66-67 71-72 71-75
  72-73 73-74 74-75 79-80 79-83 80-81 81-82 82-83 87-88 87-91 88-89 89-90
  90-91 95-96 95-100 96-97 97-98 98-99 99-100 102-103 102-107 103-104
104 - 105 \quad 105 - 106 \quad 106 - 107 \quad 113 - 114 \quad 113 - 117 \quad 114 - 115 \quad 115 - 116 \quad 116 - 117 \quad 118 - 119
118 - 122 \quad 119 - 120 \quad 120 - 121 \quad 121 - 122 \quad 123 - 124 \quad 123 - 128 \quad 124 - 125 \quad 125 - 126 \quad 126 - 127
127-128
exact/norm bonds :
5-7 6-9 7-8 8-9 8-10 11-12 11-15 13-14 13-16 23-24 23-27 24-25 25-26
26-27 \quad 30-31 \quad 30-34 \quad 31-32 \quad 32-33 \quad 33-34 \quad 57-58 \quad 59-60 \quad 61-62 \quad 63-64 \quad 63-67 \quad 64-65 \quad 64-6
65-66 \quad 66-67 \quad 69-70 \quad 71-72 \quad 71-75 \quad 72-73 \quad 73-74 \quad 74-75 \quad 77-78 \quad 79-80 \quad 79-83 \quad 80-81
81 - 82 \quad 82 - 83 \quad 85 - 86 \quad 87 - 88 \quad 87 - 91 \quad 88 - 89 \quad 89 - 90 \quad 90 - 91 \quad 93 - 94 \quad 109 - 110 \quad 111 - 112
113-114 \quad 113-117 \quad 114-115 \quad 115-116 \quad 116-117 \quad 118-119 \quad 118-122 \quad 119-120 \quad 120-121
121-122
exact bonds :
10-11 \quad 10-13 \quad 20-57 \quad 24-61 \quad 31-59 \quad 65-69 \quad 74-77 \quad 81-85 \quad 91-93 \quad 96-111 \quad 104-109
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22 36-37
102 - 103 \quad 102 - 107 \quad 103 - 104 \quad 104 - 105 \quad 105 - 106 \quad 106 - 107 \quad 123 - 124 \quad 123 - 128 \quad 124 - 125
125-126 126-127 127-128
G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9]
G2:[*10],[*11],[*12],[*13],[*14],[*15]
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom
30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 36:Atom 37:Atom 38:Atom 39:Atom
40:Atom 41:Atom 43:Atom 44:Atom 45:Atom 47:Atom 48:Atom 49:Atom
50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 57:CLASS 58:CLASS 59:CLASS 60:CLASS
 61:CLASS 62:CLASS 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:CLASS
70:CLASS 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 77:CLASS 78:CLASS 79:Atom
80:Atom 81:Atom 82:Atom 83:Atom 85:CLASS 86:CLASS 87:Atom 88:Atom 89:Atom
90:Atom 91:Atom 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom
100:Atom 102:Atom 103:Atom 104:Atom 105:Atom 106:Atom 107:Atom 109:CLASS
110:CLASS 111:CLASS 112:CLASS 113:Atom 114:Atom 115:Atom 116:Atom 117:Atom
118:Atom 119:Atom 120:Atom 121:Atom 122:Atom 123:Atom 124:Atom 125:Atom
126:Atom 127:Atom 128:Atom
L9
                STRUCTURE UPLOADED
=> d 19
L9 HAS NO ANSWERS
1.9
                                 STR
```

Structure attributes must be viewed using STN Express query preparation.

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

=> s 19

SAMPLE SEARCH INITIATED 14:31:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 31 TO ITERATE

100.0% PROCESSED 31 ITERATIONS 8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 286 TO 954
PROJECTED ANSWERS: 8 TO 329

L10 8 SEA SSS SAM L9

=> d sca

L10 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3fluorophenyl)-3-[3-[hydroxy(1-methyl-1H-imidazol-2-yl)methyl]phenyl]-, hydrochloride (9CI)

MF C27 H21 F N4 O3  $\cdot$  x C1 H

●x HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L10 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]-3-(3-methylphenyl)-

MF C25 H21 F N2 O4

Absolute stereochemistry.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L10 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)-2-fluorophenyl]-

MF C24 H17 F3 N2 O4

$$\begin{array}{c|c} F & F \\ H & C = O \\ \hline NH & O & F \\ \hline OH & OH \\ \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L10 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1S)-1,3-dihydroxybutyl]phenyl]-3-(3-fluorophenyl)-

MF C26 H23 F N2 O4

Absolute stereochemistry.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L10 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-[2-butyl-3-[(1R)-1,2-dihydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)-

MF C28 H27 F N2 O4

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L10 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-[3-(2-azido-1-hydroxyethyl)phenyl]-3-(3,5difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-

MF C24 H17 F2 N5 O3

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L10 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-(3-bromophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]-

MF C24 H18 Br F N2 O4

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L10 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxybutyl)phenyl]-

MF C26 H22 F2 N2 O4

ALL ANSWERS HAVE BEEN SCANNED

=>

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chain nodes : 10 11 12 13 14 15 16 57 58 59 60 61 62 69 70 77 78 85 86 93 94 109 110 111 112 ring nodes : 1 2 3 4 5 6 7 8 9 17 18 19 20 21 22 23 24 25 26 27 30 31 32 37 38 39 40 41 43 44 45 46 47 48 49 50 51 52 53 54 63 33 34 36 64 65 66 67 71 72 73 74 75 79 80 81 82 83 87 88 89 90 91 95 96 97 98 99 100 102 103 104 105 106 107 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128

```
chain bonds :
8-10 \quad 10-11 \quad 10-13 \quad 11-12 \quad 11-15 \quad 13-14 \quad 13-16 \quad 20-57 \quad 24-61 \quad 31-59 \quad 57-58 \quad 59-60
61-62 65-69 69-70 74-77 77-78 81-85 85-86 91-93 93-94 96-111 104-109
109-110 111-112
ring bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-9 \quad 7-8 \quad 8-9 \quad 17-18 \quad 17-22 \quad 18-19 \quad 19-20 \quad 20-21
  36-41 37-38 38-39 39-40 40-41 43-44 43-48 44-45 45-46 46-47 47-48 49-50
  49-54 50-51 51-52 52-53 53-54 63-64 63-67 64-65 65-66 66-67 71-72 71-75
  72-73 73-74 74-75 79-80 79-83 80-81 81-82 82-83 87-88 87-91 88-89 89-90
  90-91 95-96 95-100 96-97 97-98 98-99 99-100 102-103 102-107 103-104
104 - 105 \quad 105 - 106 \quad 106 - 107 \quad 113 - 114 \quad 113 - 117 \quad 114 - 115 \quad 115 - 116 \quad 116 - 117 \quad 118 - 119
118 - 122 \quad 119 - 120 \quad 120 - 121 \quad 121 - 122 \quad 123 - 124 \quad 123 - 128 \quad 124 - 125 \quad 125 - 126 \quad 126 - 127
127-128
exact/norm bonds :
5-7 6-9 7-8 8-9 8-10 11-12 11-15 13-14 13-16 23-24 23-27 24-25 25-26
26-27 \quad 30-31 \quad 30-34 \quad 31-32 \quad 32-33 \quad 33-34 \quad 57-58 \quad 59-60 \quad 61-62 \quad 63-64 \quad 63-67 \quad 64-65 \quad 64-6
65-66 \quad 66-67 \quad 69-70 \quad 71-72 \quad 71-75 \quad 72-73 \quad 73-74 \quad 74-75 \quad 77-78 \quad 79-80 \quad 79-83 \quad 80-81
81 - 82 \quad 82 - 83 \quad 85 - 86 \quad 87 - 88 \quad 87 - 91 \quad 88 - 89 \quad 89 - 90 \quad 90 - 91 \quad 93 - 94 \quad 109 - 110 \quad 111 - 112
113-114 \quad 113-117 \quad 114-115 \quad 115-116 \quad 116-117 \quad 118-119 \quad 118-122 \quad 119-120 \quad 120-121
121-122
exact bonds :
10-11 \quad 10-13 \quad 20-57 \quad 24-61 \quad 31-59 \quad 65-69 \quad 74-77 \quad 81-85 \quad 91-93 \quad 96-111 \quad 104-109
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 17-18 \quad 17-22 \quad 18-19 \quad 19-20 \quad 20-21 \quad 21-22 \quad 36-37
102-103 \quad 102-107 \quad 103-104 \quad 104-105 \quad 105-106 \quad 106-107 \quad 123-124 \quad 123-128 \quad 124-125
125-126 126-127 127-128
```

G1:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7],[\*8],[\*9]

G2:[\*10],[\*11],[\*12],[\*13],[\*14],[\*15]

## Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:CLASS 70:CLASS 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 77:CLASS 78:CLASS 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 85:CLASS 86:CLASS 87:Atom 88:Atom 89:Atom 90:Atom 91:Atom 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 100:Atom 102:Atom 103:Atom 104:Atom 105:Atom 106:Atom 107:Atom 109:CLASS 110:CLASS 111:CLASS 112:CLASS 113:Atom 114:Atom 115:Atom 116:Atom 117:Atom 126:Atom 127:Atom 128:Atom 128:

# L11 STRUCTURE UPLOADED

=> s 111

SAMPLE SEARCH INITIATED 14:34:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 31 TO ITERATE

100.0% PROCESSED 31 ITERATIONS 8 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 286 TO 954
PROJECTED ANSWERS: 8 TO 329

L12 8 SEA SSS SAM L11

=>

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```
chain nodes :
10 11 12 13 14 15 16 57 58 59 60 61 62 69 70 77 78 85 86
                                                                             93 94
109 110 111 112
ring nodes :
1 2 3 4 5 6 7 8
                        9 17
                               18 19
                                       20
                                            21
                                                22
                                                    23
                                                        24
                                                            25
                                                                    27
                                                                26
                                                                        30
                                                                            31
33 34 36 37 38 39 40 41 43 44 45 46 47 48 49 50 51 52
                                                                        53 54 63
64 65 66 67 71 72 73 74
                                75 79 80 81 82
                                                   83 87 88 89 90
                                                                         91 95 96
97 98 99 100 102 103 104 105 106 107 113 114 115 116 117
                                                                         118 119
120 121 122 123 124 125 126 127 128
chain bonds :
8-10 10-11 10-13 11-12 11-15 13-14 13-16 20-57 24-61 31-59 57-58 59-60 61-62 65-69 69-70 74-77 77-78 81-85 85-86 91-93 93-94 96-111 104-109
109-110 111-112
ring bonds :
              3-4 4-5 5-6 5-7 6-9 7-8 8-9 17-18 17-22
1-2 1-6 2-3
                                                                 18-19 19-20
                                                                               20-21
              23-27 24-25 25-26 26-27 30-31 30-34
 21-22 23-24
                                                         31-32
                                                                 32-33
                                                                        33-34
                                                                               36-37
 36-41 37-38 38-39 39-40 40-41 43-44 43-48 44-45 45-46
                                                                 46-47 47-48
                                                                               49-50
 49-54 50-51 51-52 52-53 53-54 63-64 63-67 64-65 65-66
                                                                 66-67 71-72
                                                                               71 - 75
 72-73 73-74
              74-75 79-80 79-83 80-81 81-82 82-83 87-88 87-91 88-89 89-90
90-91 95-96 95-100 96-97 97-98 98-99 99-100 102-103 102-107 103-104
104 - 105 \quad 105 - 106 \quad 106 - 107 \quad 113 - 114 \quad 113 - 117 \quad 114 - 115 \quad 115 - 116 \quad 116 - 117 \quad 118 - 119
118 - 122 \quad 119 - 120 \quad 120 - 121 \quad 121 - 122 \quad 123 - 124 \quad 123 - 128 \quad 124 - 125 \quad 125 - 126 \quad 126 - 127
127-128
```

exact/norm bonds :  $5-7 \quad 6-9 \quad 7-8 \quad 8-9 \quad 8-10 \quad 10-11 \quad 10-13 \quad 11-12 \quad 11-15 \quad 13-14 \quad 13-16 \quad 23-24 \quad 23-27$  $24 - 25 \quad 25 - 26 \quad 26 - 27 \quad 30 - 31 \quad 30 - 34 \quad 31 - 32 \quad 32 - 33 \quad 33 - 34 \quad 57 - 58 \quad 59 - 60 \quad 61 - 62 \quad 63 - 64 \quad 63 -$ 63-67 64-65 65-66 66-67 69-70 71-72 71-75 72-73 73-74 74-75 77-78 79-80 79-83 80-81 81-82 82-83 85-86 87-88 87-91 88-89 89-90 90-91 93-94  $109-110 \quad 111-112 \quad 113-114 \quad 113-117 \quad 114-115 \quad 115-116 \quad 116-117 \quad 118-119 \quad 118-122$ 119-120 120-121 121-122 exact bonds : 20-57 24-61 31-59 65-69 74-77 81-85 91-93 96-111 104-109 normalized bonds :  $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 17-18 \quad 17-22 \quad 18-19 \quad 19-20 \quad 20-21 \quad 21-22 \quad 36-37$ 36-41 37-38 38-39 39-40 40-41 43-44 43-48 44-45 45-46 46-47 47-48 49-50  $49-54 \quad 50-51 \quad 51-52 \quad 52-53 \quad 53-54 \quad 95-96 \quad 95-100 \quad 96-97 \quad 97-98 \quad 98-99 \quad 99-100$  $102 - 103 \quad 102 - 107 \quad 103 - 104 \quad 104 - 105 \quad 105 - 106 \quad 106 - 107 \quad 123 - 124 \quad 123 - 128 \quad 124 - 125$ 125-126 126-127 127-128

G1:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7],[\*8],[\*9]

G2:[\*10],[\*11],[\*12],[\*13],[\*14],[\*15]

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 57:CLASS 58:CLASS 59:CLASS 60:CI 61:CLASS 62:CLASS 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:CLASS 70:CLASS 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 77:CLASS 78:CLASS 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 85:CLASS 86:CLASS 87:Atom 88:Atom 89:Atom 90:Atom 91:Atom 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 100:Atom 102:Atom 103:Atom 104:Atom 105:Atom 106:Atom 107:Atom 109:CLASS 110:CLASS 111:CLASS 112:CLASS 113:Atom 114:Atom 115:Atom 116:Atom 117:Atom 118:Atom 119:Atom 120:Atom 121:Atom 122:Atom 123:Atom 124:Atom 125:Atom 126:Atom 127:Atom 128:Atom

#### L13 STRUCTURE UPLOADED

=> s 113

SAMPLE SEARCH INITIATED 14:40:09 FILE 'REGISTRY' 31 TO ITERATE SAMPLE SCREEN SEARCH COMPLETED -

31 ITERATIONS 8 ANSWERS 100.0% PROCESSED

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\* PROJECTED ITERATIONS: 286 TO 954

8 TO PROJECTED ANSWERS: 329

L14 8 SEA SSS SAM L13

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```
chain nodes :
10 11 12 13 14 15 16 57 58 59 60 61
                                                 62 69 70 77 78 85
                                                                          86
                                                                              93
109 110 111 112
ring nodes :
1 2 3 4 5 6 7 8
                        9 17
                                18 19 20 21
                                                             25
                                                 22
                                                     23
                                                         24
                                                                 26
                                                                      27
                                                                          30
                                                                              31
33 34 36 37 38 39
                        40 41
                               43 44 45 46 47
                                                     48 49 50 51
                                                                      52
                                                                          53 54 63
64 \quad 65 \quad 66 \quad 67 \quad 71 \quad 72 \quad 73 \quad 74 \quad 75 \quad 79 \quad 80 \quad 81 \quad 82 \quad 83 \quad 87 \quad 88 \quad 89 \quad 90
97 98 99 100 102 103 104 105 106 107 113 114 115 116
                                                                     117
                                                                          118 119
120 121 122 123 124 125
                              126 127
chain bonds :
8-10 \quad 10-11 \quad 10-13 \quad 11-12 \quad 11-15 \quad 13-14 \quad 13-16 \quad 20-57 \quad 24-61 \quad 31-59 \quad 57-58 \quad 59-60
61-62 65-69 69-70 74-77 77-78 81-85 85-86 91-93 93-94 96-111 104-109
109-110 111-112
ring bonds :
              3-4 4-5 5-6 5-7 6-9 7-8 8-9 17-18
1-2 1-6 2-3
                                                          17-22
                                                                  18-19 19-20
                                                                                 20 - 21
21-22 23-24 23-27 24-25 25-26 26-27 30-31 30-34
                                                          31-32
                                                                  32-33 33-34
                                                                                 36 - 37
 36-41 37-38 38-39 39-40 40-41 43-44 43-48 44-45
                                                          45 - 46
                                                                  46-47 47-48
                                                                                 49-50
 49-54 50-51 51-52 52-53 53-54 63-64 63-67 64-65
                                                                  66-67 71-72
                                                          65-66
                                                                                 71 - 75
              74-75 79-80 79-83 80-81 81-82 82-83 87-88 87-91 88-89 89-90
       73 - 74
 72 - 73
90-91 95-96 95-100 96-97 97-98 98-99 99-100 102-103 102-107 103-104
127-128
exact/norm bonds :
5-7 6-9 7-8 8-9 8-10 10-11 10-13 11-12 11-15 13-14 13-16 20-57 23-24
23 - 27 \quad 24 - 25 \quad 24 - 61 \quad 25 - 26 \quad 26 - 27 \quad 30 - 31 \quad 30 - 34 \quad 31 - 32 \quad 31 - 59 \quad 32 - 33 \quad 33 - 34 \quad 57 - 58
59-60 61-62 63-64 63-67 64-65 65-66 65-69 66-67 69-70 71-72 71-75 72-73
73-74 74-75 74-77 77-78 79-80 79-83 80-81 81-82 81-85 82-83 85-86 87-88
87-91 \quad 88-89 \quad 89-90 \quad 90-91 \quad 91-93 \quad 93-94 \quad 96-111 \quad 104-109 \quad 109-110 \quad 111-112
113-114 \quad 113-117 \quad 114-115 \quad 115-116 \quad 116-117 \quad 118-119 \quad 118-122 \quad 119-120 \quad 120-121
```

121-122

normalized bonds :

G1:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7],[\*8],[\*9]

G2: [\*10], [\*11], [\*12], [\*13], [\*14], [\*15]

G3:0,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:CLASS 70:CLASS 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 77:CLASS 78:CLASS 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 85:CLASS 86:CLASS 87:Atom 88:Atom 89:Atom 90:Atom 91:Atom 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 102:Atom 103:Atom 104:Atom 105:Atom 106:Atom 107:Atom 109:CLASS 110:CLASS 111:CLASS 112:CLASS 113:Atom 114:Atom 115:Atom 116:Atom 117:Atom 118:Atom 119:Atom 120:Atom 121:Atom 122:Atom 123:Atom 124:Atom 125:Atom 126:Atom 127:Atom 128:Atom 128:Atom

## L15 STRUCTURE UPLOADED

=> s 115

SAMPLE SEARCH INITIATED 14:42:44 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 31 TO ITERATE

100.0% PROCESSED 31 ITERATIONS 8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 286 TO 954

PROJECTED ANSWERS: 8 TO 329

L16 8 SEA SSS SAM L15

=> s 115 sss full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SEARCH INITIATED 14:43:07 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 547 TO ITERATE

100.0% PROCESSED 547 ITERATIONS 160 ANSWERS SEARCH TIME: 00.00.01

L17 160 SEA SSS FUL L15

=> d sca

L17 160 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3fluorophenyl)-3-[3-(hydroxy-2-pyridinylmethyl)phenyl]-

MF C28 H20 F N3 O3

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L17 160 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3fluorophenyl)-3-[3-(1-hydroxy-3-oxobutyl)phenyl]-

MF C26 H21 F N2 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L17 160 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-[3-(2-amino-1-hydroxyethyl)phenyl]-3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-

MF C24 H19 F2 N3 O3

$$\begin{array}{c|c} OH \\ H_2N-CH_2-CH \\ \hline \\ H \\ C-C \\ \hline \\ NH \\ O \end{array}$$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L17 160 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3fluorophenyl)-3-[3-[(1R)-1,2,3-trihydroxybutyl]phenyl]-

MF C26 H23 F N2 O5

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L17 160 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenepropanamide, 3-[3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxopropyl]- $\alpha$ , $\beta$ -dihydroxy-N,N-dimethyl-

MF C27 H23 F2 N3 O5

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L17 160 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-[3-[(1R)-2-chloro-1-hydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)-

MF C24 H18 C1 F N2 O3

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file zcaplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 224.76 227.40

FULL ESTIMATED COST

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ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 117T.18 3 L17

=> file registry COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 227.47 FULL ESTIMATED COST

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http://www.cas.org/support/stngen/stndoc/properties.html

=> s 117 not caplus/lc 67160240 CAPLUS/LC 4 L17 NOT CAPLUS/LC T.19

L19 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-[1,3-dihydro-5-(3-pyridinylmethoxy)-2H-benzimidazol-2ylidene]-1-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-3-(3methoxyphenyl)-

MF C31 H26 F N3 O6

CI COM

Absolute stereochemistry.

Double bond geometry unknown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L19 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3-fluorophenyl)-3-[3-[hydroxy(1-methyl-1H-imidazol-2-yl)methyl]phenyl]-

MF C27 H21 F N4 O3

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L19 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3fluorophenyl)-3-[3-(hydroxy-2-pyridinylmethyl)phenyl]-

MF C28 H20 F N3 O3

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L19 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Glycine, N,N-dimethyl-, 2-[3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)-1,3-dioxopropyl]phenyl]-2-hydroxyethyl ester

MF C28 H26 F N3 O5

CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> analyze 119 1-4 lc FIELD CODE OR DATA NOT PRESENT IN ANSWERS SPECIFIED. The answers processed either do not include the specified field or do not contain any data that may be selected from the specified field.

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=> analyze 119 1-4
ENTER DISPLAY CODE (CHEM) OR ?:1c
FIELD CODE OR DATA NOT PRESENT IN ANSWERS SPECIFIED.
The answers processed either do not include the specified field or do
not contain any data that may be selected from the specified field.
=> analyze 119
ENTER ANSWER NUMBER OR RANGE (1-):1-4
ENTER DISPLAY CODE (CHEM) OR ?:chem
L20
          ANALYZE L19 1-4 CHEM:
=> d
           ANALYZE L19 1-4 CHEM:
L20
                                      4 TERMS
TERM # # OCC # DOC % DOC CHEM
_____ ___
           1 25.00 871221-89-5
                  1 25.00 871300-52-6
    2
           1
                  1 25.00 871300-53-7
           1
    3
           1 25.00 871300-53-7
    4
****** END OF L20***
=> analyze 119 1-4 ?
Enter one or more codes from the following list.
AF ----- Alternate Molecular Formula
AR ----- Alternate Registry Number
CCI ---- Component Substance Class Identifier
CHEM ---- CAS Registry Numbers and Selected Names
CI ----- Substance Class Identifier
CMF ---- Component Molecular Formulas
{\tt CN} ----- Chemical Names (Up to 50)
CRN ---- Component Registry Numbers
DEF ---- Definition
DR ----- Deleted Registry Number
EA ----- Elemental Analysis for Ring System
ES ----- Elemental Sequence for Ring System
FCN ---- All Chemical Names
FS ---- File Segment
IN ----- CA Index Name
LC ----- CAS Registry Number Locator
MF ----- Molecular Formula
NAME ---- Selected Substance Names
PCT ---- Polymer Class Term
PR ----- Preferred Registry Number
PN ----- Patent Number
RF ---- Ring System Formula
RID ---- Ring Identifier
RL---- CAplus Super roles
RLD ---- CAplus Super roles for non-specific Derivatives
RL.NP --- Roles from Non-patents
RL.P ---- Roles from Patents
RLD.NP -- Roles for non-specific derivatives from Non-patents
RLD.P --- Roles for non-specific derivatives from Patents
RLS ---- All CAplus Super roles
RLS.NP -- CAplus Super roles - Non-patents
RLS.P --- CAplus Super roles - Patents
RN ----- CAS Registry Number
RR ----- Replacing Registry Number
SCN ---- Short Chemical Name (IN and OTHER NAMES)
SEQ ---- Protein Sequence Display using 1 Letter Amino Acid Codes (default)
SEQ3 ---- Protein Sequence Display using 3 Letter Amino Acid Codes
```

```
SQEFP --- Protein Sequence (exact family search form)
SQEN ---- Nucleic Acid Sequence (exact search form)
SQEP ---- Protein Sequence (exact search form)
SQSFP --- Protein Sequence (subsequence family search form)
SQSN ---- Nucleic Acid Sequence (subsequence search form)
SQSP ---- Protein Sequence (subsequence search form)
SR ----- Source of Registration
SZ ----- Size for Ring System
TAGS ---- Experimental Tags (same as ETAG)
ENTER DISPLAY CODE (CHEM) OR ?:LC
FIELD CODE OR DATA NOT PRESENT IN ANSWERS SPECIFIED.
The answers processed either do not include the specified field or do
not contain any data that may be selected from the specified field.
=> analyze 119 1-4 pd
'PD' IS NOT A VALID FIELD CODE FOR FILE 'REGISTRY'
The following are valid field codes:
AF ----- Alternate Molecular Formula
AR ----- Alternate Registry Number
CCI ---- Component Substance Class Identifier
CHEM ---- CAS Registry Numbers and Selected Names
CI ----- Substance Class Identifier
CMF ---- Component Molecular Formulas
CN ----- Chemical Names (Up to 50)
CRN ---- Component Registry Numbers
DEF ---- Definition
DR ----- Deleted Registry Number
EA ----- Elemental Analysis for Ring System
ES ----- Elemental Sequence for Ring System
FCN ---- All Chemical Names
FS ----- File Segment
IN ----- CA Index Name
LC ----- CAS Registry Number Locator
MF ---- Molecular Formula
NAME ---- Selected Substance Names
PCT ---- Polymer Class Term
PR ----- Preferred Registry Number
PN ----- Patent Number
RF ----- Ring System Formula
RID ---- Ring Identifier
RL---- CAplus Super roles
RLD ---- CAplus Super roles for non-specific Derivatives
RL.NP --- Roles from Non-patents
RL.P ---- Roles from Patents
RLD.NP -- Roles for non-specific derivatives from Non-patents
RLD.P --- Roles for non-specific derivatives from Patents
RLS ---- All CAplus Super roles
RLS.NP -- CAplus Super roles - Non-patents
RLS.P --- CAplus Super roles - Patents
RN ----- CAS Registry Number
RR ----- Replacing Registry Number
SCN ---- Short Chemical Name (IN and OTHER NAMES)
SEQ ---- Protein Sequence Display using 1 Letter Amino Acid Codes (default)
SEQ3 ---- Protein Sequence Display using 3 Letter Amino Acid Codes
SQEFP --- Protein Sequence (exact family search form)
SQEN ---- Nucleic Acid Sequence (exact search form)
SQEP ---- Protein Sequence (exact search form)
SQSFP --- Protein Sequence (subsequence family search form)
SQSN ---- Nucleic Acid Sequence (subsequence search form)
SQSP ---- Protein Sequence (subsequence search form)
SR ----- Source of Registration
SZ ----- Size for Ring System
```

TAGS ---- Experimental Tags (same as ETAG)
ENTER DISPLAY CODE (CHEM) OR ?:LC
FIELD CODE OR DATA NOT PRESENT IN ANSWERS SPECIFIED.
The answers processed either do not include the specified field or do not contain any data that may be selected from the specified field.

=> file zcaplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 26.19 253.66

FULL ESTIMATED COST

FILE 'ZCAPLUS' ENTERED AT 14:52:41 ON 06 JUL 2009
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FILE COVERS 1907 - 6 Jul 2009 VOL 151 ISS 2
FILE LAST UPDATED: 5 Jul 2009 (20090705/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

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This file contains CAS Registry Numbers for easy and accurate substance identification.

## => d 118

L18 ANSWER 1 OF 3 ZCAPLUS COPYRIGHT 2009 ACS on STN

AN 2006:1065682 ZCAPLUS

DN 145:419141

- TI Preparation of dihydrobenzimidazole moiety-containing propane-1,3-dione derivatives as GnRH receptor antagonists
- IN Hirano, Masaaki; Kinoyama, Isao; Matsumoto, Shunichiro; Kawaminami, Eiji; Ohnuki, Kei; Yamamoto, Hirofumi; Osoda, Kazuhiko; Takahashi, Tatsuhisa; Shin, Takashi; Koike, Takanori; Shimada, Itsuro; Hisamichi, Hiroyuki; Kusayama, Toshiyuki
- PA Astellas Pharma Inc., Japan
- SO PCT Int. Appl., 118pp. CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	WO 2006106812	A1	20061012	WO 2006-JP306641	20060330		

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            KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
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    EP 1864976
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                                                                  20060330
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    JP 2005-353577
                         Α
                               20051207
    WO 2006-JP306641
                         W
                               20060330
    MARPAT 145:419141
             THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
             ALL CITATIONS AVAILABLE IN THE RE FORMAT
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=> d 118 ibib hitstr 2-3
THE ESTIMATED COST FOR THIS REQUEST IS 7.78 U.S. DOLLARS

L18 ANSWER 2 OF 3 ZCAPLUS COPYRIGHT 2009 ACS on STN

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) / N: y

ACCESSION NUMBER: 2005:1314083 ZCAPLUS

DOCUMENT NUMBER: 144:51576

TITLE: Preparation of benzimidazole derivatives as GnRH

receptor antagonists

INVENTOR(S): Hirano, Masaaki; Kawaminami, Eiji; Kinoyama, Isao;

Matsumoto, Shunichiro; Ohnuki, Kei; Obitsu, Kazuyoshi;

Kusayama, Toshiyuki

PATENT ASSIGNEE(S): Astellas Pharma Inc., Japan

SOURCE: PCT Int. Appl., 76 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND DATE		APPLICATION NO.						DATE				
				_												
WO 2005118556			A1 20051215		WO 2005-JP10184				20050602							
W:	ΑE,	AG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
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	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	KP,	KR,	KΖ,
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	NG,	NΙ,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,
	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,
	ZA,	ZM,	ZW													
RW	: BW,	GH,	GM,	KΕ,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
	AZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,	IS,	ΙΤ,	LT,	LU,	MC,	NL,	PL,	PT,

RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG AU 2005250273 20051215 AU 2005-250273 20050602 A 1 CA 2568590 20050602 CA 2005-2568590 Α1 20051215 EP 2005-745730 20050602 EP 1752452 20070214 Α1 20071212 EP 1752452 Α9 AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR CN 1964950 20070516 CN 2005-80018280 20050602 Α BR 2005011796 20080115 BR 2005-11796 20050602 Α ZA 2006010129 20080130 ZA 2006-10129 20050602 Α RU 2347781 20090227 RU 2006-142689 C2 20050602 US 20090018177 Α1 20090115 US 2006-588485 20060804 IN 2006KN03481 Α 20070615 IN 2006-KN3481 20061122 KR 2007023715 20070228 KR 2006-725345 20061201 Α KR 882366 20090205 В1 MX 2006014131 20070307 MX 2006-14131 20061204 Α NO 2007000074 NO 2007-74 20070302 20070104 Α PRIORITY APPLN. INFO.: JP 2004-166486 20040604 Α JP 2005-99815 20050330 Α WO 2005-JP10184 W 20050602

OTHER SOURCE(S): MARPAT 144:51576

IT 871220-08-5P

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation of benzimidazole derivs. as GnRH receptor antagonists for treatment of prostate cancer, breast cancer, etc.)

RN 871220-08-5 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

IT 871222-65-0P 871224-54-3P

RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzimidazole derivs. as GnRH receptor antagonists for treatment of prostate cancer, breast cancer, etc.)

RN 871222-65-0 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1S)-1,2-dihydroxyethyl]phenyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 871224-54-3 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.

IT 871220-17-6P 871222-57-0P 871222-64-9P 871222-66-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of benzimidazole derivs. as GnRH receptor antagonists for treatment of prostate cancer, breast cancer, etc.)

RN 871220-17-6 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871222-57-0 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(hydroxymethyl)phenyl]- (CA INDEX NAME)

RN 871222-64-9 ZCAPLUS

CN 1,3-Propanedione, 1-[3-[(acetyloxy)methyl]phenyl]-3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)- (CA INDEX NAME)

RN 871222-66-1 ZCAPLUS

CN 1,3-Propanedione, 1-[3-(2-amino-1-hydroxyethyl)phenyl]-3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} \\ \text{H}_2\text{N}-\text{CH}_2-\text{CH} \\ \\ \text{H} \\ \text{C}-\text{C} \\ \\ \text{NH} \\ \text{O} \end{array}$$

ΙT 871220-09-6P 871220-10-9P 871220-11-0P 871220-13-2P 871220-15-4P 871220-19-8P 871220-21-2P 871220-23-4P 871220-25-6P 871220-27-8P 871220-29-0P 871220-31-4P 871220-33-6P 871220-35-8P 871220-37-0P 871220-39-2P 871220-41-6P 871220-43-8P 871220-45-0P 871220-47-2P 871220-49-4P 871220-51-8P 871220-53-0P 871220-55-2P 871220-57-4P 871220-59-6P 871220-61-0P 871220-63-2P 871220-65-4P 871220-67-6P 871220-69-8P 871220-71-2P 871220-73-4P 871220-75-6P 871220-77-8P 871220-79-0P 871220-81-4P 871220-83-6P 871220-85-8P 871220-87-0P 871220-89-2P 871220-91-6P 871220-93-8P 871220-95-0P 871220-97-2P 871220-99-4P 871221-01-1P 871221-03-3P 871221-05-5P 871221-07-7P 871221-09-9P 871221-11-3P 871221-13-5P 871221-15-7P 871221-17-9P 871221-19-1P 871221-21-5P 871221-23-7P 871221-25-9P 871221-27-1P 871221-29-3P 871221-31-7P 871221-33-9P 871221-35-1P 871221-37-3P 871221-39-5P 871221-41-9P 871221-43-1P 871221-45-3P 871221-47-5P 871221-49-7P 871221-51-1P 871221-53-3P 871221-55-5P 871221-59-9P 871221-69-1P 871221-71-5P 871221-73-7P 871221-75-9P 871221-77-1P 871221-79-3P 871221-81-7P 871221-83-9P 871221-85-1P 871221-87-3P 871221-90-8P 871221-92-0P 871221-94-2P 871221-96-4P 871221-98-6P 871222-00-3P 871222-02-5P 871222-04-7P 871222-06-9P 871222-08-1P 871222-10-5P 871222-12-7P 871222-14-9P 871222-16-1P 871222-18-3P 871222-20-7P 871222-21-8P 871222-22-9P 871222-23-0P 871222-24-1P 871222-26-3P 871222-28-5P 871222-30-9P 871222-32-1P 871222-34-3P 871222-36-5P 871222-38-7P 871222-40-1P 871222-41-2P 871222-42-3P 871222-43-4P 871222-44-5P 871222-45-6P 871222-46-7P 871222-47-8P 871222-48-9P 871222-49-0P 871222-50-3P 871222-51-4P 871222-52-5P 871222-53-6P 871222-54-7P 871222-55-8P 871222-56-9P 871222-58-1P 871222-59-2P 871222-60-5P 871222-62-7P 871222-63-8P 871222-67-2P 871222-68-3P 871222-69-4P 871222-70-7P 871222-71-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzimidazole derivs. as GnRH receptor antagonists for treatment of prostate cancer, breast cancer, etc.)

RN 871220-09-6 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-[3-fluoro-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 871220-10-9 ZCAPLUS

CN 1,3-Propanedione, 1-(3-chloro-5-fluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-11-0 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(3,4,5-trifluorophenyl)- (CA INDEX NAME)

RN 871220-13-2 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-3-[3-(1,2-dihydroxyethyl)phenyl]-2-(5-fluoro-1,3-dihydro-2H-benzimidazol-2-ylidene)- (CA INDEX NAME)

RN 871220-15-4 ZCAPLUS

CN 1,3-Propanedione, 2-(5,6-difluoro-1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3,5-difluorophenyl)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-19-8 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-dichlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-21-2 ZCAPLUS

CN 1,3-Propanedione, 1-(3,4-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-23-4 ZCAPLUS

CN 1,3-Propanedione, 1-(2,6-dichloro-4-pyridinyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

HO-CH<sub>2</sub>-CH
$$\begin{array}{c} OH \\ CH_2-CH \\ CH$$

RN 871220-25-6 ZCAPLUS

CN 1,3-Propanedione, 1-(2,6-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-27-8 ZCAPLUS

CN 1,3-Propanedione, 2-(5-chloro-6-fluoro-1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3,5-difluorophenyl)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-29-0 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(4-fluorophenyl)- (CA INDEX NAME)

RN 871220-31-4 ZCAPLUS

CN 1,3-Propanedione, 1-(3-chloro-5-fluorophenyl)-3-[3-(1,2-dihydroxyethyl)phenyl]-2-(5-fluoro-1,3-dihydro-2H-benzimidazol-2-ylidene)-(CA INDEX NAME)

RN 871220-33-6 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(3-methoxyphenyl)- (CA INDEX NAME)

RN 871220-35-8 ZCAPLUS

CN 1,3-Propanedione, 1-(3-chloro-4-fluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 871220-37-0 ZCAPLUS

CN Benzonitrile, 4-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]-1,3-dioxopropyl]- (CA INDEX NAME)

RN 871220-39-2 ZCAPLUS

CN 1,3-Propanedione, 1-(3-bromo-5-fluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-41-6 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[5-(1,2-dihydroxyethyl)-2-fluorophenyl]- (CA INDEX NAME)

RN 871220-43-8 ZCAPLUS

CN 1,3-Propanedione, 1-(2-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-45-0 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(3-thienyl)- (CA INDEX NAME)

RN 871220-47-2 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(3,5-dimethylphenyl)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} \\ \text{HO-CH}_2\text{-CH} \\ \\ \text{H} \\ \text{C-C} \\ \\ \text{NH} \\ \text{O} \end{array} \\ \begin{array}{c} \text{Me} \\ \\ \text{Me} \\ \\ \text{Me} \\ \end{array}$$

RN 871220-49-4 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(2,3-dimethylphenyl)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} \\ \text{HO-CH}_2\text{-CH} \\ \\ \text{C-C} \\ \text{NH} \\ \text{O} \\ \text{Me} \\ \end{array}$$

RN 871220-51-8 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(3-fluoro-4-pyridinyl)- (CA INDEX NAME)

RN 871220-53-0 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(2-thienyl)- (CA INDEX NAME)

RN 871220-55-2 ZCAPLUS

CN 1,3-Propanedione, 2-(5-chloro-1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3,5-difluorophenyl)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-57-4 ZCAPLUS

CN 1,3-Propanedione, 2-(5-chloro-6-fluoro-1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3-chloro-5-fluorophenyl)-3-[3-(1,2-dihydroxyethyl)phenyl]-(CA INDEX NAME)

RN 871220-59-6 ZCAPLUS

CN Benzoic acid, 3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]-1,3-dioxopropyl]-, methyl ester (CA INDEX NAME)

RN 871220-61-0 ZCAPLUS

CN 1,3-Propanedione, 1-(5-chloro-2-methylphenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-63-2 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(3-fluoro-4-methylphenyl)- (CA INDEX NAME)

RN 871220-65-4 ZCAPLUS

CN 1,3-Propanedione, 1-(3-chloro-5-fluorophenyl)-2-(5,6-difluoro-1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-67-6 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-[6-(trifluoromethyl)-3-pyridinyl]- (CA INDEX NAME)

RN 871220-69-8 ZCAPLUS

CN Benzenesulfonamide, 3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]-1,3-dioxopropyl]-N,N-dimethyl- (CA INDEX NAME)

RN 871220-71-2 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)-2-fluorophenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} F & & F \\ H & & C & O \\ \hline N & & C & C \\ \hline N & & C & C \\ \hline & & CH-CH_2-OH \\ \hline & & CH-CH_2-OH \\ \hline \end{array}$$

RN 871220-73-4 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)-4-fluorophenyl]- (CA INDEX NAME)

RN 871220-75-6 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)-5-fluorophenyl]- (CA INDEX NAME)

RN 871220-77-8 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(5-fluoro-2-methoxyphenyl)- (CA INDEX NAME)

RN 871220-79-0 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(3-fluoro-2-methylphenyl)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \\ \text{HO-CH}_2\text{-CH} & \\ \text{H} & \text{C-C} \\ \text{NH} & \text{O} \end{array}$$

RN 871220-81-4 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(3-methylphenyl)- (CA INDEX NAME)

RN 871220-83-6 ZCAPLUS

CN 1,3-Propanedione, 1-(4-chloro-3-fluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-85-8 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-[4-fluoro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 871220-87-0 ZCAPLUS

CN Benzonitrile, 3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]-1,3-dioxopropyl]- (CA INDEX NAME)

RN 871220-89-2 ZCAPLUS

CN 1,3-Propanedione, 1-(3-bromo-4-fluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-91-6 ZCAPLUS

CN 1,3-Propanedione, 1-(3,4-dichlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} \\ & \text{C1} \\ & \text{C1} \\ & \text{C2} \\ & \text{C3} \\ & \text{C4} \\ & \text{C4}$$

RN 871220-93-8 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(2,3,5-trifluorophenyl)- (CA INDEX NAME)

RN 871220-95-0 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-phenyl- (CA INDEX NAME)

RN 871220-97-2 ZCAPLUS

CN 1,3-Propanedione, 1-(3-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871220-99-4 ZCAPLUS

CN 1,3-Propanedione, 1-(4-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871221-01-1 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(2-methylphenyl)- (CA INDEX NAME)

RN 871221-03-3 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(4-methylphenyl)- (CA INDEX NAME)

RN 871221-05-5 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)-2-fluorophenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-07-7 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)-4-fluorophenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-09-9 ZCAPLUS

CN 1,3-Propanedione, 1-(2-chloro-5-fluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871221-11-3 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)phenyl]-3-(2-fluorophenyl)- (CA INDEX NAME)

RN 871221-13-5 ZCAPLUS

CN 1,3-Propanedione, 1-(2,3-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871221-15-7 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyethyl)-2,4-difluorophenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-17-9 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[hydroxy(1-hydroxycyclopropyl)methyl]phenyl]- (CA INDEX NAME)

RN 871221-19-1 ZCAPLUS

CN Benzenepropanoic acid, 3-[3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxopropyl]- $\alpha$ , $\beta$ -dihydroxy-, ethyl ester (CA INDEX NAME)

RN 871221-21-5 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2,3-trihydroxypropyl)phenyl]- (CA INDEX NAME)

RN 871221-23-7 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3-fluorophenyl)-3-[3-[hydroxy(1-hydroxycyclopropyl)methyl]phenyl]- (CA INDEX NAME)

RN 871221-25-9 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxy-2-methylpropyl)phenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-27-1 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxypropyl)phenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-29-3 ZCAPLUS

CN Benzenepropanenitrile,  $3-[2-(1,3-\text{dihydro}-2H-\text{benzimidazol}-2-\text{ylidene})-3-(3-\text{fluorophenyl})-1,3-\text{dioxopropyl}]-\alpha,\beta-\text{dihydroxy}-$  (CA INDEX NAME)

RN 871221-31-7 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxy-2-phenylethyl)phenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-33-9 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxy-3-methylbutyl)phenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-35-1 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxy-3-methoxypropyl)phenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-37-3 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxybutyl)phenyl]- (CA INDEX NAME)

RN 871221-39-5 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[3-(dimethylamino)-1,2-dihydroxypropyl]phenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-41-9 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxyhexyl)phenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-43-1 ZCAPLUS

CN 1,3-Propanedione, 1-[3-(2-cyclohexyl-1,2-dihydroxyethyl)phenyl]-3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)- (CA INDEX NAME)

RN 871221-45-3 ZCAPLUS

CN 1,3-Propanedione, 1-[3-(2-cyclopropyl-1,2-dihydroxyethyl)phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-47-5 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-(1,2-dihydroxypropyl)-2-fluorophenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-49-7 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3-fluorophenyl)-3-[3-(3,3,3-trifluoro-1,2-dihydroxypropyl)phenyl]- (CA INDEX NAME)

RN 871221-51-1 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[4-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871221-53-3 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-3-[4-(1,2-dihydroxyethyl)phenyl]-2-(5-fluoro-1,3-dihydro-2H-benzimidazol-2-ylidene)- (CA INDEX NAME)

RN 871221-55-5 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[2-(1,2-dihydroxyethyl)phenyl]- (CA INDEX NAME)

RN 871221-59-9 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxy-1-methylethyl)phenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} Me \\ HO-CH_2-C \\ OH \\ C-C \\ NH \\ O \end{array}$$

RN 871221-69-1 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]phenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-71-5 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1S)-1,3-dihydroxypropyl]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871221-73-7 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871221-75-9 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871221-77-1 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-2-methylphenyl]- (CA INDEX NAME)

RN 871221-79-3 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-3-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 871221-81-7 ZCAPLUS

CN 1,3-Propanedione, 1-[2-butyl-3-[(1R)-1,2-dihydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871221-83-9 ZCAPLUS

CN 1,3-Propanedione, 1-(3-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]- (CA INDEX NAME)

RN 871221-85-1 ZCAPLUS

CN 1,3-Propanedione, 1-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-2-(5-fluoro-1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 871221-87-3 ZCAPLUS

CN Benzonitrile, 3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-1,3-dioxopropyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871221-90-8 ZCAPLUS

CN 1,3-Propanedione, 2-[1,3-dihydro-5-(3-pyridinylmethoxy)-2H-benzimidazol-2-ylidene]-1-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-3-(3-methoxyphenyl)-, ethanedioate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 871221-89-5 CMF C31 H26 F N3 O6

Absolute stereochemistry.

Double bond geometry unknown.

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 871221-92-0 ZCAPLUS

CN 1,3-Propanedione, 1-(2-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-2-methylphenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871221-94-2 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-3-(3-methylphenyl)- (CA INDEX NAME)

RN 871221-96-4 ZCAPLUS

CN 1,3-Propanedione, 1-[2-chloro-3-[(1R)-1,2-dihydroxyethyl]phenyl]-3-(3-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871221-98-6 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-3-(2-methylphenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-00-3 ZCAPLUS

CN 1,3-Propanedione, 1-(2-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]- (CA INDEX NAME)

RN 871222-02-5 ZCAPLUS

CN 1,3-Propanedione, 1-(3-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-04-7 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-methoxyphenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871222-06-9 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-methylphenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-08-1 ZCAPLUS

CN 1,3-Propanedione, 1-[2-chloro-3-[(1R)-1,2-dihydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-10-5 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]- (CA INDEX NAME)

RN 871222-12-7 ZCAPLUS

CN 1,3-Propanedione, 1-(3-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-2-methylphenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-14-9 ZCAPLUS

CN 1,3-Propanedione, 1-(2-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-16-1 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-methylphenyl]-3-(3-methylphenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-18-3 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-3-(3-methoxyphenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-20-7 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-methylphenyl]-3-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-21-8 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-3-(2-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-22-9 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-methylphenyl]-3-(2-fluorophenyl)- (CA INDEX NAME)

RN 871222-23-0 ZCAPLUS

CN 1,3-Propanedione, 1-[2-chloro-3-[(1R)-1,2-dihydroxyethyl]phenyl]-3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-24-1 ZCAPLUS

CN 1,3-Propanedione, 1-(4-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-26-3 ZCAPLUS

CN 1,3-Propanedione, 1-[2-chloro-3-[(1R)-1,2-dihydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-methylphenyl)- (CA INDEX NAME)

RN 871222-28-5 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-30-9 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]-3-(3-pyridinyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-32-1 ZCAPLUS

CN 1,3-Propanedione, 1-[2-chloro-3-[(1R)-1,2-dihydroxyethyl]phenyl]-3-(4-chlorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)- (CA INDEX NAME)

RN 871222-34-3 ZCAPLUS

CN 1,3-Propanedione, 1-[2-chloro-3-[(1R)-1,2-dihydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-36-5 ZCAPLUS

CN 1,3-Propanedione, 1-[2-chloro-3-[(1R)-1,2-dihydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(2-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-38-7 ZCAPLUS

CN Benzonitrile, 3-[3-[2-chloro-3-[(1R)-1,2-dihydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxopropyl]- (CA INDEX NAME)

RN 871222-40-1 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]-3-(3-methylphenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-41-2 ZCAPLUS

CN 1,3-Propanedione, 1-(3-bromophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]- (CA INDEX NAME)

RN 871222-42-3 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[1-hydroxy-2-(methylsulfonyl)ethyl]phenyl]- (CA INDEX NAME)

RN 871222-43-4 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1S)-1,3-dihydroxybutyl]phenyl]-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871222-44-5 ZCAPLUS

CN 1,3-Propanedione, 1-[3-[(1R)-2-chloro-1-hydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-45-6 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1S)-1-hydroxyethyl]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-46-7 ZCAPLUS

CN 1,3-Propanedione, 1-[3-[(1R)-2-(acetyloxy)-1-hydroxyethyl]phenyl]-3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)- (CA INDEX NAME)

RN 871222-47-8 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-2-(dimethylamino)-1-hydroxyethyl]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-48-9 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1-hydroxy-2-(methylthio)ethyl]phenyl]- (CA INDEX NAME)

RN 871222-49-0 ZCAPLUS

CN 1,3-Propanedione, 1-[3-[(1R)-2-(acetyloxy)-1,3-dihydroxybutyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-50-3 ZCAPLUS

CN Propanoic acid, 2-methyl-, 2-[3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)-1,3-dioxopropyl]phenyl]-2-hydroxyethyl ester (CA INDEX NAME)

RN 871222-51-4 ZCAPLUS

CN Benzenepropanamide, 3-[3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxopropyl]- $\alpha$ , $\beta$ -dihydroxy-N,N-dimethyl- (CA INDEX NAME)

RN 871222-52-5 ZCAPLUS

CN 1,3-Propanedione, 1-[3-[1,2-bis(acetyloxy)ethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871222-53-6 ZCAPLUS

CN Propanoic acid, 2-methyl-, 1-[3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)-1,3-dioxopropyl]phenyl]-1,2-ethanediyl ester (9CI) (CA INDEX NAME)

RN 871222-54-7 ZCAPLUS

CN 1,3-Propanedione, 1-[3-[2-(acetyloxy)-1-hydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871222-55-8 ZCAPLUS

CN Glycine, N, N-dimethyl-, 2-[3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)-1,3-dioxopropyl]phenyl]-2-hydroxyethyl ester, hydrochloride (9CI) (CA INDEX NAME)

•x HCl

RN 871222-56-9 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3-fluorophenyl)-3-[3-(hydroxymethyl)phenyl]- (CA INDEX NAME)

RN 871222-58-1 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3-fluorophenyl)-3-[3-[(1R)-1,2,3-trihydroxybutyl]phenyl]- (CA INDEX NAME)

RN 871222-59-2 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[5-[(1S)-1,2-dihydroxyethyl]-2-thienyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 871222-60-5 ZCAPLUS

CN Benzenepropanoic acid, 3-[3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxopropyl]- $\alpha$ , $\beta$ -dihydroxy-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

RN 871222-62-7 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3-fluorophenyl)-3-[3-(hydroxy-2-pyridinylmethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 871222-63-8 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3-fluorophenyl)-3-[3-[hydroxy(1-methyl-1H-imidazol-2-yl)methyl]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

•x HCl

RN 871222-67-2 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-5-hydroxy-2H-1)

benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-2-fluorophenyl]- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 871222-68-3 ZCAPLUS

CN Acetamide, N-[2-[3-[3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxopropyl]phenyl]-2-hydroxyethyl]- (CA INDEX NAME)

RN 871222-69-4 ZCAPLUS

CN Carbonic acid, 2-[3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)-1,3-dioxopropyl]phenyl]-2-hydroxyethyl ethyl ester (CA INDEX NAME)

RN 871222-70-7 ZCAPLUS

CN 1,3-Propanedione, 1-[3-[1-(acetyloxy)-2-hydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871222-71-8 ZCAPLUS

CN Glycine, N,N-dimethyl-, 2-(acetyloxy)-2-[3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)-1,3-dioxopropyl]phenyl]ethyl ester (CA INDEX NAME)

IT 871224-52-1 871224-53-2 871224-55-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of benzimidazole derivs. as GnRH receptor antagonists for treatment of prostate cancer, breast cancer, etc.)

RN 871224-52-1 ZCAPLUS

CN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[1-hydroxy-2-(methylthio)ethyl]phenyl]- (CA INDEX NAME)

$$\begin{array}{c|c} F & F \\ H & C = O \\ \hline N & C - C \\ \hline N H & O \\ \hline O & CH-CH_2-SMe \\ \hline O & OH \\ \end{array}$$

RN 871224-53-2 ZCAPLUS

CN 1,3-Propanedione, 1-[3-[2-(acetyloxy)-1,3-dihydroxybutyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

RN 871224-55-4 ZCAPLUS

CN 1,3-Propanedione, 1-[3-(2-azido-1-hydroxyethyl)phenyl]-3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)- (CA INDEX NAME)

$$\begin{array}{c|c} F & F \\ H & C = O \\ \hline NH & C - C \\ \hline OH & OH \\ \end{array}$$

IT 871223-25-5P 871224-02-1P 871224-09-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzimidazole derivs. as GnRH receptor antagonists for treatment of prostate cancer, breast cancer, etc.)

RN 871223-25-5 ZCAPLUS

CN Benzoic acid, 3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-ethenylphenyl)-1,3-dioxopropyl]-, methyl ester (CA INDEX NAME)

$$H_2C = CH$$
 $C = O$ 
 $C = OMe$ 
 $O$ 
 $O$ 

RN 871224-02-1 ZCAPLUS

CN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3-fluorophenyl)-3-[3-(1-hydroxy-3-oxobutyl)phenyl]- (CA INDEX NAME)

RN 871224-09-8 ZCAPLUS

CN 1,3-Propanedione, 1-[3-[(acetyloxy)methyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)- (CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 3 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:31423 ZCAPLUS

DOCUMENT NUMBER: 136:102388

TITLE: Preparation of 2-(benzoazolidinylene)propane-1,3-dione

derivatives as GnRH receptor antagonists

INVENTOR(S): Hirano, Masaaki; Kawaminami, Eiji; Toyoshima, Akira;

Moritomo, Hiroyuki; Seki, Norio; Wakayama, Ryutaro;

Okada, Minoru; Kusayama, Toshiyuki

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 70 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIND		DATE		APPLICATION NO.						DATE			
WO	WO 2002002533			A1	20020110			,	WO 2	001-	20010704							
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		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KR,	KΖ,	LC,	LK,	LR,	LS,	
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		DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	ΙΤ,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	
		ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GW,	$\mathrm{ML}_{m{\prime}}$	MR,	ΝE,	SN,	TD,	ΤG			

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EP	13003	398			В1	B1 20060405												
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ES	22614	137			Т3	20061116 ES 2001-949914							20010704					
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US	69605	91			В2	2005												
KR	74829	94			В1	2007	KR 2003-700111						20030104					
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								1	US	2002-	3116	88	1	A3 2	20021	219		

OTHER SOURCE(S): MARPAT 136:102388

IT 388594-80-7P 388595-01-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (benzoazolidinylene)propanedione derivs. as GnRH receptor antagonists for treating sex hormone-dependent diseases)

RN 388594-80-7 ZCAPLUS

CN Benzoic acid, 3,3'-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxo-1,3-propanediyl]bis-, dimethyl ester (9CI) (CA INDEX NAME)

RN 388595-01-5 ZCAPLUS

CN Benzoic acid, 3-[2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1,3-dioxo-3-phenylpropyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \parallel \\ C - Ph \\ \downarrow \\ C - C \\ \parallel \\ O \end{array}$$

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS

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=> file registry
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 10.29 263.95

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109 110 111 112
ring nodes :
1 2 3 4 5 6 7 8
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33 34 36 37 38 39
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64 \quad 65 \quad 66 \quad 67 \quad 71 \quad 72 \quad 73 \quad 74 \quad 75 \quad 79 \quad 80 \quad 81 \quad 82 \quad 83 \quad 87 \quad 88 \quad 89 \quad 90
97 98 99 100 102 103 104 105 106 107 113 114 115 116
                                                                       117
120 121 122 123 124 125
                               126 127
chain bonds :
8-10 \quad 10-11 \quad 10-13 \quad 11-12 \quad 11-15 \quad 13-14 \quad 13-16 \quad 20-57 \quad 24-61 \quad 31-59 \quad 57-58 \quad 59-60
61-62 65-69 69-70 74-77 77-78 81-85 85-86 91-93 93-94 96-111 104-109
109-110 111-112
ring bonds :
               3-4 4-5 5-6 5-7 6-9 7-8 8-9 17-18
1-2 1-6 2-3
                                                             17-22
                                                                    18-19 19-20
21-22 23-24 23-27 24-25 25-26 26-27 30-31 30-34
                                                             31-32
                                                                    32-33 33-34
                                                                                    36 - 37
 36-41 37-38 38-39 39-40 40-41 43-44 43-48 44-45
                                                             45 - 46
                                                                    46-47 47-48
                                                                                    49-50
 49-54 50-51 51-52 52-53 53-54 63-64 63-67 64-65
                                                                    66-67 71-72
                                                             65-66
                                                                                    71 - 75
               74-75 79-80 79-83 80-81 81-82 82-83 87-88 87-91 88-89 89-90
       73 - 74
 72-73
90-91 95-96 95-100 96-97 97-98 98-99 99-100 102-103 102-107 103-104
127-128
exact/norm bonds :
5-7 \quad 6-9 \quad 7-8 \quad 8-9 \quad 8-10 \quad 10-11 \quad 10-13 \quad 11-12 \quad 11-15 \quad 13-14 \quad 13-16 \quad 20-57 \quad 23-24
23 - 27 \quad 24 - 25 \quad 24 - 61 \quad 25 - 26 \quad 26 - 27 \quad 30 - 31 \quad 30 - 34 \quad 31 - 32 \quad 31 - 59 \quad 32 - 33 \quad 33 - 34 \quad 57 - 58
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73-74 74-75 74-77 77-78 79-80 79-83 80-81 81-82 81-85 82-83 85-86 87-88
87-91 \quad 88-89 \quad 89-90 \quad 90-91 \quad 91-93 \quad 93-94 \quad 96-111 \quad 104-109 \quad 109-110 \quad 111-112
113-114 \quad 113-117 \quad 114-115 \quad 115-116 \quad 116-117 \quad 118-119 \quad 118-122 \quad 119-120 \quad 120-121
121-122
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chain nodes :

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normalized bonds:

1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22 36-37 36-41 37-38 38-39 39-40 40-41 43-44 43-48 44-45 45-46 46-47 47-48 49-50 49-54 50-51 51-52 52-53 53-54 95-96 95-100 96-97 97-98 98-99 99-100 102-103 102-107 103-104 104-105 105-106 106-107 123-124 123-128 124-125 125-126 126-127 127-128

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9]

G2:[*10],[*11],[*12],[*13],[*14],[*15]

G3:0,S

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom
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Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom
30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 36:Atom 37:Atom 38:Atom 39:Atom
40:Atom 41:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom
50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 57:CLASS 58:CLASS 59:CLASS 60:CLASS
61:CLASS 62:CLASS 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:CLASS
70:CLASS 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 77:CLASS 78:CLASS 79:Atom
80:Atom 81:Atom 82:Atom 83:Atom 85:CLASS 86:CLASS 87:Atom 88:Atom 89:Atom
90:Atom 91:Atom 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom 109:CLASS
110:CLASS 111:CLASS 112:CLASS 113:Atom 114:Atom 115:Atom 116:Atom 117:Atom

100:Atom 102:Atom 103:Atom 104:Atom 105:Atom 106:Atom 107:Atom 109:CLASS 110:CLASS 111:CLASS 112:CLASS 113:Atom 114:Atom 115:Atom 116:Atom 117:Atom 118:Atom 119:Atom 120:Atom 121:Atom 122:Atom 123:Atom 124:Atom 125:Atom 126:Atom 127:Atom 128:Atom

## L21 STRUCTURE UPLOADED

=> s 121 SAMPLE SEARCH INITIATED 15:04:15 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 78 TO ITERATE

100.0% PROCESSED 78 ITERATIONS 8 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 1031 TO 2089

PROJECTED ITERATIONS: 1031 TO 2089
PROJECTED ANSWERS: 8 TO 329

L22 8 SEA SSS SAM L21

=> d sca

L22 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-(3-fluorophenyl)-3-[3-[hydroxy(1-methyl-1H-imidazol-2-yl)methyl]phenyl]-, hydrochloride (9CI)
MF C27 H21 F N4 O3 . x Cl H

●x HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L22 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]-3-(3-methylphenyl)-

MF C25 H21 F N2 O4

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L22 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-(1,2-dihydroxyethyl)-2-fluorophenyl]-

MF C24 H17 F3 N2 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L22 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-1-[3-[(1S)-1,3-dihydroxybutyl]phenyl]-3-(3-fluorophenyl)-

MF C26 H23 F N2 O4

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L22 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-[2-butyl-3-[(1R)-1,2-dihydroxyethyl]phenyl]-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-(3-fluorophenyl)-

MF C28 H27 F N2 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L22 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1,3-Propanedione, 1-[3-(2-azido-1-hydroxyethyl)phenyl]-3-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-

MF C24 H17 F2 N5 O3

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L22 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN 1.3-Propanedione, 1-(3-bromophenyl)-2-(1,3-dihydro-2F

1,3-Propanedione, 1-(3-bromophenyl)-2-(1,3-dihydro-2H-benzimidazol-2-ylidene)-3-[3-[(1R)-1,2-dihydroxyethyl]-4-fluorophenyl]-

MF C24 H18 Br F N2 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L22 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Propanedione, 1-(3,5-difluorophenyl)-2-(1,3-dihydro-2H-benzimidazol-2ylidene)-3-[3-(1,2-dihydroxybutyl)phenyl]MF C26 H22 F2 N2 O4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file zcaplus
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 2.40 266.35

FILE 'ZCAPLUS' ENTERED AT 15:06:37 ON 06 JUL 2009

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FILE COVERS 1907 - 6 Jul 2009 VOL 151 ISS 2
FILE LAST UPDATED: 5 Jul 2009 (20090705/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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8.77 275.12

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Property values tagged with IC are from the  ${\tt ZIC/VINITI}$  data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 JUL 2009 HIGHEST RN 1160791-26-3 DICTIONARY FILE UPDATES: 5 JUL 2009 HIGHEST RN 1160791-26-3

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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LOGOFF? (Y)/N/HOLD:y

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STN INTERNATIONAL LOGOFF AT 15:38:48 ON 06 JUL 2009